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NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 26	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27	Oct 21	EVENTLINE has been reloaded
NEWS 28	Oct 24	BEILSTEIN adds new search fields
NEWS 29	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 31	Nov 18	DKILIT has been renamed APOLLIT
NEWS 32	Nov 25	More calculated properties added to REGISTRY
NEWS 33	Dec 02	TIBKAT will be removed from STN
NEWS 34	Dec 04	CSA files on STN
NEWS 35	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36	Dec 17	TOXCENTER enhanced with additional content
NEWS 37	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 38	Dec 30	ISMEC no longer available
NEWS 39	Jan 13	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40	Jan 21	NUTRACEUT offering one free connect hour in February 2003
NEWS 41	Jan 21	PHARMAML offering one free connect hour in February 2003
NEWS 42	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 43	Feb 13	CANCERLIT is no longer being updated
NEWS 44	Feb 24	METADEX enhancements

NEWS 45 Feb 24 PCTGEN now available on STN
NEWS 46 Feb 24 TEMA now available on STN
NEWS 47 Feb 26 NTIS now allows simultaneous left and right truncation
NEWS 48 Feb 26 PCTFULL now contains images
NEWS 49 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results

NEWS EXPRESS January 6 CURRENT WINDOWS VERSION IS V6.01a,
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AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
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FILE CONTENT:1907 - 16 Mar 2003 VOL 138 ISS 11

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> s nitration reaction

```
          5698 NITRATION
        273267 REACTION
L2          28 NITRATION REACTION
               (NITRATION(W)REACTION)

=> s l2 and microreactor
            55 MICROREACTOR
L3           0 L2 AND MICROREACTOR

=> s l2 and micro?
          5864 MICRO?
L4           1 L2 AND MICRO?

=> dis l4 bib abs


L4   ANSWER 1 OF 1  CASREACT  COPYRIGHT 2003 ACS
AN   113:23454  CASREACT
TI   FK409, a novel vasodilator isolated from the acid-treated fermentation
     broth of Streptomyces griseosporeus.  III.  Reaction mechanism and
     synthesis
AU   Hino, Motohiro; Takase, Shigehiro; Itoh, Yoshikuni; Uchida, Itsuo;
     Okamoto, Masanori; Kohsaka, Masanobu; Aoki, Hatsuo; Imanaka, Hiroshi
CS   Explor. Res. Lab., Fujisawa Pharm. Co., Ltd., Tsukuba, 300-26, Japan
SO   Journal of Antibiotics (1989), 42(11), 1589-92
     CODEN: JANTAJ; ISSN: 0021-8820
DT   Journal
LA   English
AB   FK409 [(E)-O2NCHMeCEt:CHC(:NOH)CONH2, I] was considered to be formed via a
     novel synchronous nitrosation-nitration reaction of
     FR-900411 [(2E,4E)-MeCH:CEtCH:CHCONH2, II] under acidic conditions with
     nitrite formed by microbial redn. of nitrate.  Total synthesis
     of I was achieved starting from (E)-2-ethyl-2-butenal via a nitrosation
     reaction of II as a key step.


=> s l2 and pd<august 1999
        361432 PD<AUGUST 1999
               (PD<19990800)
L5          26 L2 AND PD<AUGUST 1999

=> s l5 not l4
L6          25 L5 NOT L4

=> dis l5 1-25  bib abs


L5   ANSWER 1 OF 26  CASREACT  COPYRIGHT 2003 ACS
AN   132:151343  CASREACT
TI   A study of the reaction of different phenol substrates with nitric oxide
     and peroxynitrite
AU   Yenes, Susana; Messeguer, Angel
CS   Department of Biological Organic Chemistry, IIQAB (CSIC), Barcelona,
     08034, Spain
SO   Tetrahedron (1999), 55(49), 14111-14122
     CODEN: TETRAB; ISSN: 0040-4020
PB   Elsevier Science Ltd.
DT   Journal
LA   English
GI
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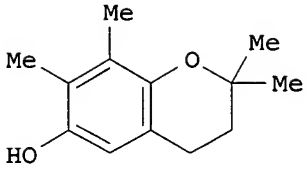
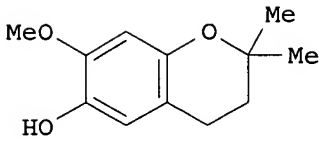
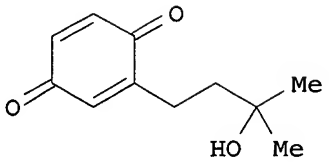


I



II



III

AB The reactivity of different phenol substrates, e.g., 4-ClC6H4OH, with nitric oxide and peroxynitrite was investigated. In general, nitration is the major reaction with peroxynitrite, while reactions with aq. solns. of nitric oxide led to mixts. of nitro and nitroso derivs. depending upon the phenol. Nitrosation occurs on phenol substrates bearing a free para-position with respect to the OH group with the exception of 1-naphthol, which afforded a 1:1 mixt. of the 2- and the 4-nitroso derivs. Chromans I and II showed the highest reactivity with peroxynitrite, which suggests that they can act as efficient scavengers of this toxic intermediate. In both cases the corresponding 5-nitro deriv. was the only reaction product detected. Finally, the fact that chroman II reacts with nitric oxide to afford the p-quinone deriv. III in 90% yield suggests that this antioxidant could also be of potential use as specific nitric oxide tracer in biol. tissues.

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 130:209610 CASREACT
TI Furopyridines. XXVIII. Reactions of 3-bromo derivatives of furo[2,3-b]-, -[3,2-b]-, -[2,3-c]- and -[3,2-c]pyridine and their N-oxides
AU Yamaguchi, Seiji; Awajima, Kazuaki; Hirai, Yoshiro; Yokoyama, Hajime; Shiotani, Shunsaku
CS Department of Chemistry, Faculty of Science, Toyama University, Toyama, 930, Japan
SO Journal of Heterocyclic Chemistry (**1998**), 35(6), 1249-1255
CODEN: JHTCAD; ISSN: 0022-152X
PB HeteroCorporation
DT Journal
LA English
AB Bromination of 3-bromofuro[2,3-b]pyridine, 3-bromofuro[3,2-b]pyridine and 3-bromofuro[3,2-c]pyridine afforded the 2,3-dibromo derivs., while 3-bromofuro[2,3-c]-pyridine did not give the dibromo deriv. Nitration of these compds. gave 2-nitro-3-bromo compds. The N-oxides of the title compds. were submitted to the cyanation with trimethylsilyl cyanide to yield corresponding .alpha.-cyanopyridine compds. Chlorination of bromofuropyridines with phosphorus oxychloride gave chloropyridine derivs. or chlorofuran derivs. Acetoxylation of bromofuropyridine oxides with acetic anhydride yielded acetoxypyridine compds.

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 130:196745 CASREACT
TI 2-Nitroferrocenyloxazolines: precursors to nitrofulvalenes and derivatives of (pS)- and (pR)-2-aminoferrocenecarboxylic acids
AU Salter, Rhys; Pickett, Tom E.; Richards, Christopher J.
CS Department of Chemistry, Cardiff University, Cardiff, CF1 3TB, UK
SO Tetrahedron: Asymmetry (**1998**), 9(23), 4239-4247
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier Science Ltd.
DT Journal
LA English
AB Diastereoselective lithiation of (S)-2-ferrocenyl-4-(1-methylethyl)oxazoline, followed by addn. of N2O4, gave (S)-2-[(pS)-2-nitroferrocenyl]-4-(1-methylethyl)oxazoline which was subsequently converted into derivs. of (pS)-2-aminoferrocenecarboxylic acid. The corresponding (pR)-derivs. were obtained through use of a removable TMS blocking group. The 2-nitroferrocenyloxazolines produced in this work underwent facile photo-decomplexation to give 2-nitrocyclopentadienyliden-1,3-oxazolidenes.
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 128:167195 CASREACT
TI Reactions of bridged halosubstituted adamantane derivatives with nitric acid
AU Klimochkin, Yu. N.; Leonova, M. V.; Moiseev, I. K.; Aleksandrov, A. M.
CS Samara State Technical University, Samara, 443056, Russia
SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (**1997**), 33(3), 340-344
CODEN: RJOCEQ; ISSN: 1070-4280
PB MAIK Nauka/Interperiodica Publishing
DT Journal
LA English
AB Reactions of bridged halosubstituted adamantane derivs. with nitric acid result in nitrolysis products. In the presence of acetic anhydride, the reactions proceed at nodal positions to form nitroxy derivs., while in the case of 2,2-dichloroadamantane, the formation of a 1,4,4-trichloro-substituted deriv. is obsd. The nitroxylation of 2-fluoroadamantane results in the formation of predominantly products with the cis-configuration.
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 128:167194 CASREACT
TI Nitroxylation of 2-substituted adamantane derivatives
AU Klimochkin, Yu. N.; Leonova, M. V.; Moiseev, I. K.
CS Samara State Technical University, Samara, 443056, Russia
SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (**1997**), 33(3), 334-339
CODEN: RJOCEQ; ISSN: 1070-4280
PB MAIK Nauka/Interperiodica Publishing
DT Journal
LA English

AB The reactions of bridged alkyladamantanes with nitric acid result in a mixt. of 1,2-nitroxy and 1,4-nitroxy, hydroxy, and nitro derivs., while nitroxylation of compds. with electron-withdrawing substituents in the bridging position gives only the corresponding 5-nitroxy derivs. Substituted adamantanes were characterized by the predominant formation of products with a Z-configuration. The comparative reactivity of 2-substituted adamantane derivs. in the reactions with nitric acid was detd. Correlations between logkapp of the nitroxylation of 2-R-adamantanes and the induction Taft .sigma.*-consts. were established.
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 125:114649 CASREACT
TI syntheses and activities of 6-heterocyclyl-1-(substituted phenyl)benzotriazole herbicidal agents
IN Condon, Michael E.; Crews, Alvin D., Jr.; Manfredi, Mark C.
PA American Cyanamid Co., USA
SO U.S., 38 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5523277	A	19960604	US 1995-387140	19950210
	US 5496954	A	19960305	US 1995-437099	19950505
	US 5545742	A	19960813	US 1995-437112	19950505
	ZA 9600901	A	19970805	ZA 1996-901	19960205
PRAI	US 1995-387140	19950210			

OS MARPAT 125:114649
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A multistep process for the synthesis of a 6-heterocyclyl-1-(substituted phenyl)benzotriazole having the structural formula I comprises the condensation of [(benzotriazolyl)phenoxy]propionate, e.g., II [e.g., R1 = OCHMeCO2Me (1), OMe, OCF3, NMe2, Me] [in which II were prepd. from cyclocondensation of Me 2-[p-(acetamido-2-amino-4-fluoroanilino)phenoxy]propionate and Na nitrite] with 3,4,5,6-tetrahydrophthalic anhydride (2). E.g., a soln. of 1 and 2 in HOAc is refluxed for 24 h to give 6-heterocyclyl-1-(substituted phenyl)benzotriazole III. (Phenyl)benzotriazoles I (e.g., III) were tested for herbicidal activity which comprised applying the compd. to the foliage of the plants or to the soil or H2O contg. seeds or other propagating organs thereof at a rate of .apprx.0.016 kg/ha to 4.0 kg/ha.

L5 ANSWER 7 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 124:342842 CASREACT
TI Nitration of benzene to dinitrobenzene and mononitrobenzene using anhydrous nitric acid in the absence of sulfuric acid or aprotic dipolar solvent
IN Mason, Robert W.
PA Olin Corp., USA

SO U.S., 4 pp., Cont.-in-part of U.S. 5,354,924.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5488187	A	19960130	US 1994-290575	19940815
	US 5354924	A	19941011	US 1993-108035	19930817
PRAI	US 1988-210549	19880622			
	US 1993-108035	19930817			
	US 1992-900213	19920617			

AB A process is claimed for nitrating benzene to produce dinitrobenzene by a liq. phase **nitration reaction** of anhyd. nitric acid (designate nitric acid having an acid concn. of between 95 and 100 wt. %, preferably at least 98 wt. %, the remainder being water) with benzene in a reactor at a reaction temp. of between 30.degree. and 70.degree., and a reaction pressure not exceeding atm. pressure, said reaction employing a molar ratio of nitric acid plus any water to benzene of between 15:1 and 25:1, said reaction being conducted in the absence of sulfuric acid, and in the absence of any aprotic dipolar solvent during the reaction and in the absence of any aprotic dipolar solvent to halt the reaction, to produce said dinitrobenzene in a product mixt., followed by vacuum distn. of the product mixt., in the absence of any aprotic dipolar solvent, to remove unreacted nitric acid from said product mixt. thereby providing a dinitrobenzene product. In another aspect, the present invention relates to a process for nitrating benzene to produce mononitrobenzene by a liq. phase **nitration reaction** of anhyd. nitric acid with benzene in a reactor at a reaction temp. of between 0.degree. and 60.degree., and a reaction pressure not exceeding atm. pressure, for a reaction time that is preferably less than 15 (more preferably less than 5) minutes, said reaction employing a molar ratio of nitric acid plus any water to benzene of between 2:1 and 4:1, said reaction being conducted in the absence of sulfuric acid, and in the absence of any aprotic dipolar solvent as described above. The following illustrates dinitration: a magnetically stirred soln. of 55.07 g (0.857 mol) of 98% nitric acid in a 100 mL flask was chilled in a water bath; benzene (3.71 g, 0.048 mol) was injected subsurface to the nitric acid at 0.75 mL/min (mol ratio of nitric acid plus water to benzene = 18:1); extn. with CH_2Cl_2 followed by GC anal. indicated complete conversion in < 1 h (mononitrobenzene content < 200 ppm, trinitrophenol content of 200 ppm) and dinitrobenzene isomer ratio 1,2:1,3:1,4 = 9.6:88.3:2.0. The following illustrates mononitration: to a 4 mL glass vial was fed 7.0 mL of 98 % HNO_3 (10.5 g, 0.163 mol of HNO_3) and 5.0 mL benzene (4.39 g, 0.056 mol of benzene) at feed rates of 0.22 mL/min and 0.135 mL/min, resp.; the reactor content was adjusted to 2 mL (mean reaction residence time of 2.8 min); the reactor water bath was maintained at 15.degree. (.+-. 5.degree.); extn. with CH_2Cl_2 was followed by GC anal. which indicated recovery of 0.047 mol (83 %) of nitrobenzene.

L5 ANSWER 8 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 123:169503 CASREACT
TI Method for producing aminocarbazole derivatives
IN Kamikawa, Taku; Maruyama, Osamu
PA Sumitomo Chemical Co, Japan
SO Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 07133261	A2	19950523	JP 1993-282636	19931111
PRAI	JP 1993-282636	19931111			

AB Aminocarbazole derives., useful as intermediates for dyes or pigments, are prepd. by catalytic hydrogenation of nitrocarbazoles in the presence of Fe-contg. Ni (1-40 wt.% Fe-Ni) catalyst and an alkali in an inert solvent. The preferred nitrocarbazole derivs. are 1- or 3-nitro-9-(lower alkyl)carbazoles. This process can directly use nitrocarbazole derivs. isolated by regular procedures from a **nitration reaction** mixt. and the redn. is not interfered and slowed down by impurities such as NO3 ions in the raw material nitrocarbazole derivs. and thereby does not result in low yields. Thus, 100 g 9-ethylcarbazole was nitrated by concd. HNO3 in 245 g o-dichlorobenzene and the reaction mixt. was neutralized with 10% aq. NaOH, followed by sepg. the oil layer and washing it with warm water to give a soln. (370 g) contg. 110.0 g 3-nitro-9-ethylcarbazole (90% yield), 8.0 g 1-nitro-9-ethylcarbazole, and NO3- 30 ppm in o-dichlorobenzene. The latter soln. 375, H2O 115, NaOH 1.0, and Raney Ni (30 wt.% Fe) 2.2 g were added to an autoclave, hydrogenated under H pressure 8 kg/cm2.G at 80.degree. with stirring for 3 h, cooled to 70.degree., and filtered to give, after sepn. of the aq. layer, a soln. (345 g) of 3-amino-9-ethylcarbazole in o-dichlorobenzene in 98% yield. Hydrogenation of the same soln. in the presence of Raney Ni without Fe and FeSO4 at 80.degree. and H pressure 8 kg/cm2.G for 14 h gave 3-amino-9-ethylcarbazole in 87% yield.

L5 ANSWER 9 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 123:55613 CASREACT
TI Nitration by oxides of nitrogen. 9. Preparation of nitramine-nitrates by ring-opening nitration of azetidines by dinitrogen pentoxide (N2O5)
AU Golding, Peter; Millar, Ross W.; Paul, Norman C.; Richards, David H.
CS Defense Res. Agency, Kent, TN14 7BP, UK
SO Tetrahedron (**1995**), 51(17), 5073-82
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English

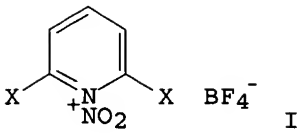
AB Eleven azetidines, bearing various types of substituents on the ring nitrogen, were treated with N2O5 in chlorinated solvents at sub-ambient temp. and in certain cases formed 1,3-nitramine-nitrate products by a novel ring-opening **nitration reaction** analogous to that established for aziridines. Yields of the nitramine-nitrates, where ring-opening took place, were generally moderate to high (41-88 %), but azetidines bearing N-acyl substituents (acetyl, butyryl or carbamyl) instead underwent nitrolysis of the exocyclic substituent to form N-nitroazetidine. Also, azetidines bearing strongly electron-withdrawing groups such as picryl were inert to attack by N2O5. The different reactivity of azetidines compared with aziridines is rationalized in terms of the reduced ring strain of the four-membered ring compds.

L5 ANSWER 10 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 122:265918 CASREACT
TI A New Route to 15N-Labeled, N-Alkyl, and N-Amino Nucleosides via N-Nitration of Uridines and Inosines
AU Ariza, Xavier; Bou, Valenti; Vilarrasa, Jaume
CS Faculty of Chemistry, University of Barcelona, Barcelona, 08028, Spain
SO Journal of the American Chemical Society (**1995**), 117(13), 3665-73

CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB A novel method for the specific [3-15N]-labeling of pyrimidine nucleosides and [1-15N]-labeling of purine nucleosides is reported. The N-**nitration reaction** is carried out in good yields with nitronium trifluoroacetate in cold dichloromethane. Treatment of the resulting N-nitro nucleosides with 15NH3, alkylamines, or hydrazine cleaves the pyrimidine ring at room temp., affording open intermediates which undergo cyclization to 15N-labeled, N-alkylated, or N-amino nucleosides, resp. Prepn. of [1-15N]adenosine from inosine in a 52% overall yield is illustrative of the scope of the procedure. [3-15N,15NH2]-5'-O-Acetyl-3-amino-2',3'-O-isopropylideneuridine and [1-15N,15NH2]-2',3',5'-tri-O-acetyl-1-aminoinosine have also been obtained from double labeled hydrazine. By using a 15N-labeled substrate and/or 15N-labeled benzylamine it is shown that the amine attack takes mainly place at C4 of uridine and at C2 of inosine.

L5 ANSWER 11 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 120:53917 CASREACT
TI Nitration by oxides of nitrogen. Part 6. Preparation of di- and polynitrates by ring-opening nitration of epoxides by dinitrogen pentoxide (N2O5)
AU Golding, Peter; Millar, Ross W.; Paul, Norman C.; Richards, David H.
CS Def. Res. Agency, Fort Halstead/Sevenoaks/Kent, TN14 7BP, UK
SO Tetrahedron (**1993**), 49(32), 7037-50
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
AB Eighteen epoxides were treated with N2O5 in chlorinated hydrocarbon solvents (principally CH2Cl2) to give vicinal nitrate ester products by a novel ring-opening **nitration reaction**. The procedure offers easier temp. control and simpler isolation procedures compared with conventional mixed-acid nitrations; it also enables selective nitrations to be carried out on polyfunctional substrates. The scope and limitations of the reaction, as well as those of an alternative route utilizing N2O4 with in situ oxidn. of an intermediate nitrite-nitrate, are discussed.

L5 ANSWER 12 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 114:228678 CASREACT
TI Aprotic nitration (NO2+BF4-, nitryl tetrafluoroborate) of 2-halo- and 2,6-dihalopyridines and transfer-nitration chemistry of their N-nitropyridinium cations
AU Duffy, Joseph L.; Laali, Kenneth K.
CS Dep. Chem., Kent State Univ., Kent, OH, 44242, USA
SO Journal of Organic Chemistry (**1991**), 56(9), 3006-9
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
GI



I

AB NO2+BF4- nitration of 2,6-dibromo- and 2,6-dichloropyridine in CH3CN results in predominant C-nitration, whereas in CH2Cl2, N-nitration is predominant. With 2,6-difluoropyridine only C-nitration is obsd. Dehalogenation of the C-nitrated derivs. affords 3-nitropyridine in moderate but greatly improved yields over conventional protic nitration of pyridine. Despite favorable steric inhibition to resonance and the -I effects of halogens, N-nitrated pyridinium salts I (X = Br, Cl) do not transfer-nitrate to aroms. even under forcing conditions. The lack of transfer-nitration reactivity is not due to in situ rearrangement of the nitro onium ions to nitrito onium ions. A mechanism involving neighboring group participation by the 2,6-halogens is proposed. The monohalo-N-nitropyridinium cations transfer-nitrate toluene and benzene. Transfer-nitration selectivities of the 2-bromo- and 2-chloro-N-nitropyridinium cations are comparable (KT/KB = 41-44), but the 2-fluoro-N-nitro cation is much less selective (more reactive) (KT/KB = 15.4), indicative of a stronger -I effect, weakening the N-N bond.

L5 ANSWER 13 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 113:23454 CASREACT
TI FK409, a novel vasodilator isolated from the acid-treated fermentation broth of Streptomyces griseosporeus. III. Reaction mechanism and synthesis
AU Hino, Motohiro; Takase, Shigehiro; Itoh, Yoshikuni; Uchida, Itsuo; Okamoto, Masanori; Kohsaka, Masanobu; Aoki, Hatsuo; Imanaka, Hiroshi
CS Explor. Res. Lab., Fujisawa Pharm. Co., Ltd., Tsukuba, 300-26, Japan
SO Journal of Antibiotics (**1989**), 42(11), 1589-92
CODEN: JANTAJ; ISSN: 0021-8820
DT Journal
LA English
AB FK409 [(E)-O2NCHMeCEt:CHC(:NOH)CONH2, I] was considered to be formed via a novel synchronous nitrosation-**nitration reaction** of FR-900411 [(2E,4E)-MeCH:CEtCH:CHCONH2, II] under acidic conditions with nitrite formed by microbial redn. of nitrate. Total synthesis of I was achieved starting from (E)-2-ethyl-2-butenal via a nitrosation reaction of II as a key step.

L5 ANSWER 14 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 112:219231 CASREACT
TI Manufacture of 1-nitroanthraquinone
IN Muszynski, Miroslaw
PA Osrodek Badawczo-Rozwojowy Przemyslu Barwnikow "Organika", Pol.
SO Pol., 4 pp.
CODEN: POXXA7
DT Patent
LA Polish
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	PL 136528	B2	19860228	PL 1983-243478	19830818

PRAI PL 1983-243478 19830818
AB The title compd. (I) is produced by nitration of a 5-50% anthraquinone (II) soln. or suspension in .gtoreq.70% H2SO4 or oleum contg. .ltoreq.65% SO3 by using a 5-50% aq. inorg. nitrate soln. at a nitrate/II mol ratio (1.0-2.5):1 and at -10 to +120.degree.. Preferably, the nitrate is NaNO3, KNO3, Ca(NO3)2, and/or Al(NO3)3. Purity of the resulting I is >90% which is satisfactory for manuf. of 1-aminoanthraquinone and further dye intermediates. Thus, the **nitration reaction** was done in a cascade of 4 reactors where a 10% II soln. in 100% H2SO4 at 20.8 parts/min and 30% aq. KNO3 soln. at 4.5 parts/min were fed into the 1st 1 m3 reactor, and in the 2nd reactor, 65% oleum was added at 5 parts/min, and in the 4th reactor, water was added at 50 parts/min, with temps. in the 1st, 2nd, 3rd, and 4th reactors 35-45.degree., 65-75.degree., 90.degree., and 30.degree., resp. The product was withdrawn, filtered on a rotary filter, washed with water to pH 7, and dried to give I (purity 93%) at 25 parts/min.

L5 ANSWER 15 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 112:51866 CASREACT
TI Structure and synthesis of FK409, a novel vasodilator isolated from Streptomyces as a semi-artificial fermentation product
AU Hino, Motohiro; Takase, Shigehiro; Itoh, Yoshikuni; Uchida, Itsuo; Okamoto, Masanori; Hashimoto, Masashi; Kohsaka, Masanobu
CS Explor. Res. Lab., Fujisawa Pharm. Co., Tsukuba, 300-26, Japan
SO Chemical & Pharmaceutical Bulletin (**1989**), 37(10), 2864-6
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
AB The structures of FK409, a semi-artificial fermn. product and its precursor 4-ethylhexa-2,4-dienamide (I), were established by chem. and spectroscopic evidence and confirmed by conversion of I to FK409 via a synchronous nitrosation-**nitration reaction**.

L5 ANSWER 16 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 111:186494 CASREACT
TI Assessment of on-line nitration reactions as a means of determining nitrate by reversed-flow injection with reductive amperometric detection at a glassy carbon electrode
AU Fogg, Arnold G.; Scullion, S. Paul; Edmonds, Tony E.
CS Chem. Dep., Loughborough Univ. Technol., Loughborough/Leicestershire, LE11 3TU, UK
SO Analyst (Cambridge, United Kingdom) (**1989**), 114(5), 579-81
CODEN: ANALAO; ISSN: 0003-2654
DT Journal
LA English
AB Five compds. were investigated for use as online reagents in concd. H2SO4 for the reductive reversed flow-injection amperometric detn. of nitrate as a nitro deriv. at a glassy carbon electrode. The H2SO4 was dild. rapidly on injecting reagent soln. into a sample carrier stream and therefore the **nitration reaction**, which generally only takes place at H2SO4 concns. of greater than about 70%, had to be rapid. Thiophene-2-carboxylic acid was found to be the most suitable reagent of those studied. The **nitration reaction** was sufficiently rapid and the first of two redn. steps was at -0.19 V vs. SCE as indicated by linear sweep voltammetry; hence the detn. was free from interference by dissolved oxygen. Problems assocd. with contamination of the electrode surface with redn. product, which caused loss of signal after making repeated injections over an extended period, remained.

L5 ANSWER 17 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 109:233186 CASREACT
TI Separation of sulfuric and nitric acids from dinitrotoluene-containing toluene **nitration reaction** mixtures by water addition
IN Witt, Harro; Beckhaus, Heiko
PA Bayer A.-G., Fed. Rep. Ger.
SO Ger. Offen., 3 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

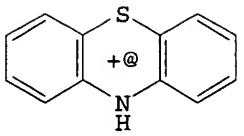
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3705091	A1	19880901	DE 1987-3705091	19870218
	EP 279312	A2	19880824	EP 1988-101799	19880208
	EP 279312	A3	19900425		
	EP 279312	B1	19920506		
	R: BE, DE, ES, FR, IT				
	ES 2031167	T3	19921201	ES 1988-101799	19880208
	US 5001286	A	19910319	US 1988-155199	19880212
	JP 63203650	A2	19880823	JP 1988-32001	19880216
	JP 2640956	B2	19970813		
PRAI	DE 1987-3705091		19870218		

AB In the manuf. of dinitrotoluene, toluene **nitration reaction** mixts., after removal of the major portion of H2SO4 and HNO3, still contain .ltoreq.5% HNO3 and .ltoreq.6% H2SO4. By addn. of .ltoreq.10% H2O (based on dinitrotoluene content) to the **nitration reaction** mixt., a phase sepn. is produced and the remainder of the acids are removed in the aq. phase.

L5 ANSWER 18 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 107:22931 CASREACT
TI Some features characterizing the **nitration reaction** of secondary polynitroalkanes
AU Eremenko, L. T.; Oreshko, G. V.; Fadeev, M. A.
CS Otd. Inst. Khim. Fiz., Chernogolovka, USSR
SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (**1986**), (6), 1357-61
CODEN: IASKA6; ISSN: 0002-3353
DT Journal
LA Russian
AB Nitration of pyridinium salts of (O2N)2CRCH2CH(NO2)CH2CR(NO2)2 (R = NO2, F) with HNO3, HNO3-H2SO4, aq. HNO3, N2O4, NO2BF4, and ClNO2 was studied. Products and product ratios varied widely with reagents and reagent concns.

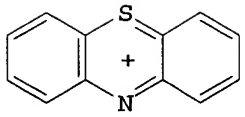
L5 ANSWER 19 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 96:6667 CASREACT
TI Oxidation state of cation radicals in the **nitration reaction** of phenothiazine by nitric acid
AU Morkovnik, A. S.; Dobaeva, N. M.; Okhlobystin, O. Yu.
CS Rostov Gos. Univ., Rostov, 344006, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (**1981**), (9), 1214-16
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian

GI



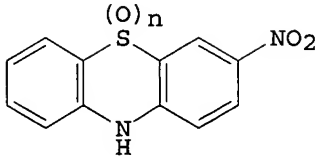
ClO_4^-

I



ClO_4^-

II



III

AB Nitration of phenothiazine by HNO3-HClO4 gave 78% cation radical I which was oxidized by HNO3 to give 68% phenothiazonium perchlorate II. Further nitration gave 81% III (n = 1) via III (n = 0).

L5 ANSWER 20 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 84:30013 CASREACT
TI Halosubstituted phenylcyclopropanes in a **nitration reaction**
AU Shabarov, Yu. S.; Mochalov, S. S.; Novokreshchennykh, V. D.; Volkov, E. M.; Ermishkina, S. A.
CS Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR
SO Zhurnal Organicheskoi Khimii (**1975**), 11(9), 1907-13
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Nitration of I in Ac2O gave 40% II, 23% III and 9% IV. Nitration of V (X = Cl, Br) gave 33-51.9% VI and 31.7-43.8% VII; nitration of V (X = iodo) gave 11.4% VI, 16.8% VII, 53% (2-nitrophenyl)cyclopropane, 5.5% 1-(2-iodophenyl)-1,3-propanediol dinitrate, and 5.4% 1-acetoxy-1-(2-iodophenyl)-3-propanol. The orientation of the NO2 was detd. by the cyclopropyl ring. Several of the cyclopropylhalonitrobenzenes were isomerized.

L5 ANSWER 21 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 84:4749 CASREACT
TI Nitration of furan derivatives by acetylnitrate. I. Products of the nitration of the methyl ester of furan-2-carboxylic acid
AU Lola, D.; Venters, K.; Liepins, E.; Hillers, S.
CS Inst. Org. Sint., Riga, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (**1975**), (7), 883-9
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Nitration of Me 2-furancarboxylate by HNO3-H2SO4-Ac2O gave I-VI which were sepd. by chromatog. and identified by ir, uv, and NMR spectroscopy.

L5 ANSWER 22 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 83:192710 CASREACT
TI Demethylation and nitration of aryldimethilamines with cerium(IV) ammonium nitrate
AU Galliani, Guido; Rindone, Bruno; Scolastico, Carlo
CS Ist. Chim. Org., Univ. Milano, Milan, Italy
SO Synthetic Communications (**1975**), 5(5), 319-23
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
AB Treatment of Me2NPh with cerium ammonium nitrate (I) in MeOH gave 40% p-Me2NC6H4C6H4NMe2-p; in HOAc or MeCN 2,4-(O2N)2C6H3NHMe was obtained in 47 and 11% yield, resp. Treatment of p-O2NC6H4NMe2 with I in MeOH, MeCN, and HOAc, resp. gave p-O2NC6H4NHMe in 89, 60, and 23% yield, resp.; similar results were obtained for p-RC6H4NMe2 in HOAc and MeCN. A mechanism was presented for the oxidative demethylation process and the **nitration reaction**.

L5 ANSWER 23 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 69:2806 CASREACT
TI Chemistry and biochemistry of plant matter. XX. Nitration of 3',4'-dimethoxyflavanone and derivatives
AU Reichel, Ludwig; Miller, Kurt
CS Humboldt Univ., Berlin, Fed. Rep. Ger.
SO Justus Liebigs Annalen der Chemie (**1968**), 712, 146-51
CODEN: JLACBF; ISSN: 0075-4617
DT Journal
LA German
AB The course of the **nitration reaction** with fuming HNO3 and the influence of various substituents on the nitration of 3',4'-dimethoxyflavanone and its derivs. was studied. A no. of substituted 2'-hydroxynitrochalcones and their corresponding nitroflavanones were prepd. and characterized.

L5 ANSWER 24 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 57:29296 CASREACT
TI Synthesis of 2,2-dinitropropanol. Studies on continuous preparation
AU Hamel, Edward E.; Dehn, John S.; Love, Joseph A.; Scigliano, Joseph J.; Swift, Arden H.
CS Aerojet-Gen. Corp., Sacramento, CA
SO Ind. Eng. Chem., Prod. Res. Develop. (**1962**), 1, 108-16
DT Journal
LA Unavailable
AB Two routes to 2,2-dinitropropanol (I) have been evaluated as potential production processes. One route utilized the oxidative-**nitration reaction** of AgNO3 and NaNO2 on MeCH:CHNO2 to produce MeCH(NO2)2 (II). Treatment of II with HCHO in the presence of a basic catalyst or treatment of its salt, MeC(NO2):NO2Na, with HCHO and 1 equiv. acid produced I. Overall yields of 75% were obtained on a pilot plant scale. Ag losses (about 1%) constituted a serious drawback to large scale production. The second method (Meer, Ann. 181, 1(1876)) involved conversion of MeCHClNO2 (III) to MeC(NO2):NO2K (IV) and methylolation of IV to give I. A satisfactory prepn. of pure III was devised and a con-tinuous 4-step process was developed for I starting with nitroethane (V) with III and IV as intermediates. Although the first method gave higher yields (80% vs. 65% based on V), the second method appeared to be superior for the prepn. of large quantities of I.

L5 ANSWER 25 OF 26 CASREACT COPYRIGHT 2003 ACS
AN 50:27961 CASREACT
TI Alkaline nitration. I. The nitration of amines with cyanohydrin nitrates
AU Emmons, Wm. D.; Freeman, Jeremiah P.
CS Rohm & Haas Co., Huntsville, AL
SO J. Am. Chem. Soc. (**1955**), 77, 4387-90
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB Me2C(CN)ONO2 (I) has been found to be a unique reagent for effecting nitration under alk. conditions. Primary and secondary amines are converted with I to the corresponding nitramines. Me2C(OH)CN (255 g.) stirred 0.5 hr. with 462 g. white fuming HNO3 (d. 1.48-1.50) in 1225 g. Ac2O, the mixt. poured into 1500 cc. ice water, stirred 1 hr. intermittently, and extd. with three 300-cc. portions CH2Cl2, and the ext. washed with 200 cc. 5% aq. NaHCO3, dried, and fractionated gave 255-67 g. I, b10 65-6.degree., nD20 1.4172. iso-Bu2NH (64.5 g.) in 100 cc. MeCN treated at room temp. with 13.0 g. I in 50 cc. MeCN, the mixt. heated 4 hrs. at 80.degree., poured into 200 cc. 10% HCl, and extd. with CH2Cl2, the ext. washed with 5% aq. NaHCO3 and H2O, dried, and evapd., and the white cryst. residue recrystd. from EtOH and H2O gave iso-Bu2NNO2, shiny white platelets, m. 79-80.degree.. Morpholine (17.4 g.) treated at room temp. with 13.0 g. I, the mixt. heated 1 hr. at 80.degree., poured into dil. HCl, and extd. with CH2Cl2, the ext. dried and evapd., and the solid residue (13.0 g.) recrystd. from EtOH and H2O yielded 10.9 g. N-nitromorpholine, m. 51-3.degree.. BuNH2 (36.5 g.) in 50 cc. MeCN treated with 13.0 g. I, the mixt. refluxed 6 hrs. and worked up in the usual manner, and the residue distd. yielded 6.1 g. BuNHNO2, b0.05 68-70.degree., nD20 1.4596; the aq. exts. made alk. with Na2CO3 and extd. with Et2O, and the ext. dried and distd. gave 5.6 g. .alpha.-butylaminoisobutyronitrile, b8 58-9.degree., nD20 1.4286. Similarly were prepd. the following nitramines (b.p./mm., nD20, and % yield given) with I: Me2NNO2, - (m. 57-8.degree.), -, 76; Et2NNO2, 50-2.degree./0.2, 1.4525, 60; Pr2NNO2, 90-2.degree./8, 1.4558, 42; Bu2NNO2 (II), 69-70.degree./0.1, 1.4562, 54; iso-Am2NNO2, 112-14.degree./2, 1.4604, 64; N-nitropiperidine, 62-4.degree./0.2, 1.4968, 62; N-nitropyrrolidine, - (m. 55-7.degree.), -, 60; PrNHNO2, 52-6.degree./0.1, 1.4610, 50; iso-BuNHNO2, 58-60.degree./0.1, 1.4570, 54; AmNHNO2, 60-2.degree./0.2, 1.4611, 55; iso-AmNHNO2, 62-4.degree./0.02, 1.4594, 54. Piperazine hexahydrate (III) (38.4 g.) in 100 cc. HCONMe2 heated 5 hrs. at 80.degree. with 13.0 g. I, the solvent distd. off in vacuo, the residue cooled in Dry Ice, and the resulting pale yellow solid filtered and recrystd. from EtOH yielded 7.0 g. small white platelets of mono-N-nitropiperazine, m. 127-8.degree.; it gave with PhNCS the phenylthiourea deriv., m. 204-5.degree. (from EtOH). III (38.4 g.) in 100 cc. EtOH and 50 cc. CH2Cl2 refluxed 4 hrs. with 13.0 g. I, the mixt. allowed to stand overnight, the solvent evapd., and the residue recrystd. from EtOH yielded 6.7 g. N,N'-di(.alpha.-cyanoisopropyl)piperazine, m. 178-80.degree.. III (19.4 g.) in 75 cc. HCONMe2 heated 4 hrs. at 75.degree. with 13.0 g. I, the mixt. evapd., and the solid residue recrystd. from EtOH yielded 6.8 g. N-nitro-N'-(.alpha.-cyanoisopropyl)piperazine, m. 140-2.degree.. Cyclohexanone cyanohydrin (90 g.), 111 g. fuming HNO3, and 180 g. Ac2O gave in the usual manner 107.5 g. cyclohexanone cyanohydrin nitrate (IV), b0.3 62-4.degree., nD20 1.4660. Cyclopentanone (168 g.), 260 g. KCN, and 377 cc. Ac2O in 500 cc. H2O yielded 183 g. cyclopentanone cyanohydrin (V), b0.3 74-6.degree.. V (183 g.), 310 g. fuming HNO3, and 837 g. Ac2O gave in the usual manner 216 g. nitrate (VI) of V, b0.25 50-1.degree., nD20 1.4592. IV (8.5 g.) and 32.3 g. Bu2NH heated 4 hrs. in 50 cc. tetrahydrofuran, the mixt. poured

into dil. HCl and extd. with Et2O, the ext. washed with 10% aq. NaHSO3, dried, and concd., and the residue distd. gave 5.0 g. II. VI (7.8 g.) and 32.3 g. Bu2NH yielded 5.5 g. II. Me2C(OH)CCl3.2H2O (21.3 g.) added during 10 min. to 102 g. Ac2O and 18.9 g. anhyd. HNO3, the mixt. stirred 0.5 hr. at room temp., quenched in 400 cc. H2O-ice mixt., and extd. with three 100-cc. portions Et2O, the ext. washed with 10% aq. Na2CO3 and H2O, dried, and evapd. in vacuo, and the residue distd. gave 20.0 g. Me2C(ONO2)CCl3, b1.0 46-50.degree., nD20 1.4810; it did not react with piperidine. Me2C(OH)CO2Et (13.2 g.) added to 18.9 g. abs. HNO3, 51 g. Ac2O, and 30 g. AcOH, the mixt. stirred 2 hrs. at room temp., poured into ice water and extd. with CH2Cl2, and the ext. dried and distd. gave 15.9 g. Me2C(ONO2)CO2Et, b12 74-6.degree., nD20 1.4172; it did not react with secondary amines.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	72.88	73.09

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